



NIST Combinatorial Methods Center

Discussion Sessions

NCMC-10, Completing the Combi Loop: Examining Persistent Challenges in Implementing Combinatorial Materials Science

Thursday, October 5, 2006 - Afternoon ♦ Bldg. 101 / Lecture Room B & Rm. B-111

Goals:

- To further examine library fabrication, system integration, and other persistent challenges to implementing Combi methods for materials.
- To produce roadmaps that outline and prioritize:
 - Technologies and approaches that address current and emerging challenges
 - Specifications for vendor supplied combinatorial and high-throughput instrumentation and software
 - Topics for future workshops and symposia at national meetings

Process:

For these discussions, Workshop attendees will divide into Teams that will rotate through three Breakout Sessions. Please be prepared to contribute to the discussions by considering the following questions and issues prior to arrival at NCMC-10, and during the Workshop technical sessions. *All reports produced from these discussions will reflect a summary message from the NCMC consortium, and will not identify the views of individual members.*

Breakout Session 1. *Technologies needed to meet your persistent challenges*

- A. What are the persistent challenges to your implementation of Combi today? What challenges to you foresee in two years? Consider, for example:
 - Design/fabrication of libraries for new materials sets. For what *types* of materials? For what kinds of processing parameters?
 - System/workflow integration. Where are your informatics “bottlenecks”?
 - Automation of existing equipment. What kinds of instruments?
 - High-throughput measurements. For what materials properties?
 - Measurement reliability. For what materials properties?
 - Database development
 - High-throughput data analysis. What kinds of data?
- B. What specific technologies are needed to meet your challenges? Consider, for example:
 - Library approaches and instrumentation
 - Measurement approaches and instrumentation
 - Informatics tools for system integration and data analysis
 - Standards and reference materials

Deliverable from Session 1: A published NCMC report with prioritized lists of key technologies needed now and in two years.

Breakout Session 2. *Vendor-supplied instrumentation and software*

- A. What Combi-related products you would be inclined to purchase if they were commercially available today? What would be your required specifications for these products? Examples to consider:
- Library fabrication equipment. For what materials systems? Over what variables? Required specifications?
 - High-throughput measurement/screening instruments. For what properties? Required tolerances and specifications?
 - Software systems. Examples:
 - For high-throughput data analysis. For what kinds of data?
 - For system integration. For what kinds of instruments/components?
 - Reference materials. For what kinds of Combi measurements?
 - Standard file formats for integration. For what kinds of instruments and data?
- B. What types of commercial instrumentation and software do you currently use for Combi? What types of currently available instruments have caught your eye? In each case, how could these products be improved? Consider, for example:
- Throughput
 - Ability to automate
 - Versatility
 - Reliability
 - System integration
 - Your key specifications for improvement
- C. What vendor companies would benefit from hearing these messages?

Deliverable from Session 2: A NCMC document outlining opportunities for vendors to develop or improve products for Combi. This report will be distributed to vendors, including those identified in 2C above, and will be posted on the NCMC Web site.

Breakout Session 3. *Workshops and national symposia*

- A. What topics should be addressed in future NCMC Workshops?
- B. What topics for Combi symposia at national conferences would draw your attendance and contribution?
- C. What emerging topics in Combi should be addressed through focused symposia at national conferences?
- D. At what national meetings would Combi symposia be useful?

Deliverable from Session 3. Your input will be reflected in plans for future NCMC Workshops and symposium proposals submitted to conference committees.